

# Some comments to the quantum fluctuation theorems

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It is demonstrated that today's quantum fluctuation theorems are component part of old quantum fluctuation-dissipation relations [Sov.Phys.-JETP 45, 125 (1977)], and typical misunderstandings in this area are pointed out.

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1. This communication is devoted to those general statistical properties of externally driven quantum systems what are due to time reversibility of their underlying (Hamiltonian) microdynamics. For the first time a complete list of such properties was suggested in item 5 in [1]. Later [2, 3] they were named “generalized fluctuation-dissipation relations” (FDR) since relate dissipation and irreversibility in (linear and non-linear) response functions to fluctuations (see also [4, 5] and references therein).

Here, I would like to comment last decade activity in this field, concerning the quantum “fluctuation theorems” (FT) [6–8], and focusing on three its aspects as follow. Firstly, that some authors surprisingly do not understand existence of two qualitatively different types of the external Hamiltonian driving. Secondly, that some recently presented relations in fact are particular cases of the old FDR. Thirdly, that the only real problem in this field is establishing of physically meaningful rules of ordering and symmetrization of quantum operators and super-operators.

2. As in [5], let us start from separation of two types of external driving. One is such that small changes of a driving “force”  $x = x(t)$  cause only small changes in any degree of freedom or part of our (now quantum) system. Another type is such that even small change in  $x$  can cause arbitrary strong changes in some degrees of freedom and thus strong energy exchange between them and the rest of the system. For example, if system represents quasi-free charge carrier with charge  $q$  in dielectric fluid (or crystal) contained in volume with diameter  $L$ , and  $x$  is electric field, then equilibrium state at any  $x = \text{const} \neq 0$  (let arbitrary small) realizes only when the carrier achieves boundary of the container while the force lowers the carrier's potential energy by  $w \sim |qx|L$  thus producing work  $w$  dissipated by the fluid (crystal).

Clearly, on one hand, free energy of this final state significantly differs from starting value (at  $x = 0$ ). On the other hand, if we are interested in the carrier's transport in itself, then both the final equilibrium state and its free energy  $F(x)$  are far from of our interest. In this case, instead, we have to consider thermodynamic limit  $L \rightarrow \infty$  (or not too long time intervals only) and thus non-equilibrium steady (or quasi-stationary) state.

Hence, the corresponding FDR characterize essentially

non-equilibrium transient process, either steady or finishing at essentially new state with different free energy. But in no way “the restricted case where there is no change in free energy” (citation from [7], p.230404-2, right column) ! Such curious view [6, 7] says about incomprehension of true contents of FDR (and hence FT) and headless reading of [1].

We see that under the second type of driving a part of the whole system (charge carrier in the above example) behaves as open system (in between of driving source and other parts may be playing role of thermostats). Therefore below for brevity let us call this case “open” while the first one “closed”. In “open” case a natural measure of violation of equilibrium by external force  $x(t)$  is its value itself while in “closed” case a value of its time derivative,  $dx(t)/dt$ . This difference can be underlined by different representations of FDR [3] (though, of course, it wipes out under sufficiently high-frequency oscillating  $x(t)$ ).

3. In [1] a unified consideration of both the “closed” and “open” cases was suggested, using division of full system's Hamiltonian,  $H(x)$ , as follows:

$$H(x) = H_0 - h(x), \quad H_0(x) = H(x_0), \quad (1)$$

$$h(x) = H(x_0) - H(x)$$

(page 127, left column in [1]). In the open case, obviously, it is reasonable to put on  $x_0 = 0$  and besides write the “perturbation Hamiltonian”  $h(x)$  in the form  $h(x) = xQ$  (although the latter is not necessary). Main relation of [1], expressed by formulae (17),(19),(21) and (23) there, is

$$\langle A_1(t_1) \dots A_n(t_n) e^{-\beta H_0(t)} e^{\beta H_0(0)} \rangle_{x(\tau)} =$$

$$= \langle \bar{A}_n(t - t_n) \dots \bar{A}_1(t - t_1) \rangle_{\epsilon x(t-\tau)}, \quad (2)$$

where  $A_j$  are arbitrary operators, the over-line means their transposition, presence of time arguments in  $A_j(t_j)$  and  $H_0(t)$  means that operators are treated in the Heisenberg picture,  $H_0(0) = H_0$ ,  $\epsilon = \pm 1$  is parity (or parities) of the driving force (or forces)  $x(t)$  in respect to time reversal, and angle brackets denote average over canonical distribution of initial conditions under given (arbitrary) trajectory of the force:

$$\langle \dots \rangle_{x(\tau)} = \text{Tr} \dots \rho_0, \quad \rho_0 = q^{-1} \exp(-\beta H_0), \quad (3)$$

with  $q$  being normalizing factor. At that, if  $H_0$  includes magnetic field (or other time-odd parameter) then

on the right in (2) it must be inverted ([1], p.129, left column). If  $A_j$  are Hermitian and possess definite parities,  $\bar{A}_j = \epsilon_j A_j$ , then (2) turns to formula (24) from [1],

$$\begin{aligned} & \langle A_1(t_1) \dots A_n(t_n) e^{-\beta H_0(t)} e^{\beta H_0(0)} \rangle_{x(\tau)} = \\ & = \epsilon_1 \dots \epsilon_n \langle A_n(t - t_n) \dots A_1(t - t_1) \rangle_{\epsilon x(t-\tau)} \end{aligned} \quad (4)$$

Formulas (2) or (4) represent complete lists of symmetry relations produced by the microscopic time reversibility and therefore can be termed “generating quantum FDR”.

4. Of course, these FDR are more comfortable in the “open” case than in ‘closed’ one (see item 2 above). Therefore, if we are ready to restrict our consideration by closed case (and thus closed systems) only, then it is suitable to replace  $H_0$  in (2)-(4) by  $H(x)$ . At that, the only additional difference from derivation of (2) and (4) on p.129 in [1] is that normalizing factor  $q$  becomes  $x$ -dependent. Repetition of the derivation yields

$$\begin{aligned} & \langle A_1(t_1) \dots A_n(t_n) e^{-\beta H(t,x(t))} e^{\beta H(0,x(0))} \rangle_{x(\tau)} = \\ & = \langle \bar{A}_n(t - t_n) \dots \bar{A}_1(t - t_1) \rangle_{\epsilon x(t-\tau)} \times \\ & \quad \times e^{\beta[F(x(0)) - F(x(t))]} , \end{aligned} \quad (5)$$

where  $H(t, x(t))$  means  $H(x(t))$  taken in the Heisenberg picture, so that  $H(0, x) = H(x)$ ,

$$\begin{aligned} & \langle \dots \rangle_{x(\tau)} = \text{Tr} \dots \rho(x(0)) , \\ & \rho(x) = q^{-1}(x) \exp(-\beta H(x)) , \end{aligned} \quad (6)$$

and  $F(x) = -\beta^{-1} \ln q(x)$ . If all  $A_j$  are Hermitian with definite parity, then

$$\begin{aligned} & \langle A_1(t_1) \dots A_n(t_n) e^{-\beta H(t,x(t))} e^{\beta H(0,x(0))} \rangle_{x(\tau)} = \\ & = \epsilon_1 \dots \epsilon_n \langle A_n(t - t_n) \dots A_1(t - t_1) \rangle_{\epsilon x(t-\tau)} \times \\ & \quad \times e^{\beta[F(x(0)) - F(x(t))]} \end{aligned} \quad (7)$$

Notice that FDR (5) and (7) can be obtained also directly from FDR (2) and (4), respectively, as their particular (“closed”) case, in full analogy with transition between two classical FT in [5]. It is sufficient, at any fixed  $t$  and  $x(t)$  to choose in (1)  $x_0 = x(t)$  and then apply identity

$$e^{-\beta H_0(t)} e^{\beta H_0} \rho_0 = \frac{q(x(0))}{q(x(t))} e^{-\beta H(t,x(t))} e^{\beta H(x(0))} \rho(x(0)) ,$$

where the above designations also are used.

5. In general, any rearrangement of operators  $A_j(t_j)$  in the relations (2), (4), (5) and (7) produces, - in contrast to the classical theory, - not identical but new relation. Therefore, any a priori prescribed re-ordering or symmetrization of these operators, in respect to their time arguments or indices, abolishes a part of information contained in initial relations and thus lowers generality of result as compared with them. Consequently, any grouping of particular FDR (2), (4), (5) or (7) into some generating relation, e.g. for some characteristic function or functional, leads to loss of information and instead of

heightening generality (as it would be in classical theory) in fact lowers it!

For example, let us make in (7) redesignation  $A_j \Rightarrow A_{k_j}$ , multiply both sides by  $\prod_{j=1}^n u_{k_j}(t_j)$ , where  $u_k(t)$  are arbitrary (complex) test functions, take sum over all  $k_j$ , integrate over all  $t_j$ , divide by  $n!$  and sum over all non-negative  $n$ . These operations can be easily performed mentally, “without paper and pencil”, producing generating FDR

$$\begin{aligned} & \langle \exp \left[ \int_0^t u_k(\tau) A_k(\tau) d\tau \right] e^{-\beta H(t,x(t))} e^{\beta H(0,x(0))} \rangle_{x(\tau)} = \\ & = \langle \exp \left[ \epsilon_k \int_0^t u_k(t - \tau) A_k(\tau) d\tau \right] \rangle_{\epsilon x(t-\tau)} \times \\ & \quad \times e^{\beta[F(x(0)) - F(x(t))]} \end{aligned} \quad (8)$$

(with summation over repeated index  $k$ ). But what it really generates (after functional differentiations by  $u_k(\tau)$ ) ? Clearly, relations for fully symmetrized quantum statistical moments only, thus losing an unknown amount of information in comparison with (7) (e.g. information from various commutators of  $A_k(t)$ ).

Hence, the above relations for arbitrary asymmetric non-ordered quantum moments are most general form of FDR. Just by this reason authors of [1] confined themselves by non-symmetrized relations (but not because they “were not able” to perform the mentioned trivial operations, as assumed in [8]). Therefore it looks strangely when authors of [7, 8] characterize relations like (8) (formula (12) from [7] or (55) from [8]) as “universal” and “most general”.

In reality, relations (8) can not generate even the Efremov’s quadratic FDT [9] or complete set of independent four-index quantum FDR [10]. If one wants to avoid loss of these results and simultaneously use fully symmetrized moments only, then the latter should be defined like it was suggested in Sec.3 in [3] (or see formula (2) in [4]).

6. Actual achievement of quantum theory in the field of FDR after [1] is not formulae like (8) but realization of those circumstance that measuring of energy difference between two system’s states requires two independent measurements of energy, therefore, operator  $H(t, x(t)) - H(0, x(0))$ , or  $H_0(t) - H_0(0)$ , is not quantum observable representing the energy difference [8].

In other words, the product of two exponentials in (2) and (4), or (5) and (7), is true quantum equivalent of classical exponentials  $\exp(-\beta E)$  or  $\exp(-\beta \mathcal{E})$ , respectively, with  $E = H_0(t) - H_0(0)$  being system’s internal energy change in the open case and  $\mathcal{E} = H(t, x(t)) - H(0, x(0))$  total energy change in the closed case.

Hence, characteristic function of energy change also must be defined by means of pair of exponentials [6, 8], for instance,

$$G(u; x(\tau)) = \langle e^{uE} \rangle_{x(\tau)} \equiv \text{Tr} e^{uH_0(t)} e^{-uH_0(0)} \rho_0 \quad (9)$$

Then, choosing in (2)  $n = 2$ ,  $A_1 = \exp(-uH_0)$ ,  $A_2 = \exp(uH_0)$ ,  $t_1 = 0$  and  $t_2 = t$ , one obtains characteristic function representation of the “quantum work FT” [6, 8]:

$$G(u - \beta; x(\tau)) = G(-u; \epsilon x(t - \tau)) \quad (10)$$

Quite similarly from (5) arises FT for the  $\mathcal{E}$ .

7. The same can be said about differences  $Q(t_f) - Q(t_i)$  of any other quantum observable (e.g. space coordinate of charge carrier in example from item 2 above). However, since generally  $Q$  does not commute with  $H_0$  and  $H(x)$ , we can not merely replace  $H_0$  in (9) by  $Q$ , but have to define a reasonable rule for ordering or/and symmetrization of operator products.

Among many formally acceptable rules there is one prompted by the correspondence principle. It states that characteristic functional of any variable (or set of variables)  $A$  can be represented (see e.g. [4] and references therein) by

$$\langle \exp \int_0^t u(\tau) A(\tau) d\tau \rangle_{x(\tau)} = \text{Tr } \rho, \quad (11)$$

where  $\rho$  is solution to equation

$$\dot{\rho} = [H(x(t)), \rho]/i\hbar + u(t) A \circ \rho, \quad (12)$$

with  $\circ$  denoting the symmetrized, or Jordan, product,  $A \circ B \equiv (AB + BA)/2$ . The corresponding rule is chronological time ordering of Jordan products:

$$\begin{aligned} & \langle \exp \int_0^t u(\tau) A(\tau) d\tau \rangle_{x(\tau)} = \\ & = \text{Tr } \overleftarrow{\exp}[\frac{1}{2} \int_0^t u(t') A(t') dt'] \rho_0 \overrightarrow{\exp}[\frac{1}{2} \int_0^t u(t') A(t') dt'] \end{aligned} \quad (13)$$

with  $\overleftarrow{\exp}$  and  $\overrightarrow{\exp}$  being chronological and anti-chronological exponents. According to this rule,

$$\langle A_1(t_1) \dots A_n(t_n) \rangle_{x(\tau)} = \text{Tr } \mathcal{T} \left[ \prod_{j=1}^n A_j(t_j) \circ \right] \rho_0, \quad (14)$$

where  $\mathcal{T}$  means chronological ordering of the Jordan products, and

$$\begin{aligned} & \langle e^{u[Q(t_f) - Q(t_i)]} \rangle_{x(\tau)} = \\ & = \text{Tr } e^{uQ(t_f)/2} e^{-uQ(t_i)/2} \rho_0 e^{-uQ(t_i)/2} e^{uQ(t_f)/2} \end{aligned} \quad (15)$$

under  $t_f > t_i \geq 0$ . Clearly, this rule relates any finite-time difference to two separate measurements. In particular, at  $Q = H_0$  (and  $t_i = 0$ ,  $t_f = t$ ) expression (15) coincides with (9).

8. Derivation of FDR under just defined ordering-symmetrization rule copies derivation of (2), (4) in [1].

For the open case, the result is

$$\begin{aligned} & \langle e^{-\beta H_0(t)} \exp \left[ \int_0^t u_k(\tau) A_k(\tau) d\tau \right] e^{\beta H_0(0)} \rangle_{x(\tau)} = \\ & = \langle \exp \left[ \int_0^t \epsilon_k u_k(t - \tau) A_k(\tau) d\tau \right] \rangle_{\epsilon x(t - \tau)} \end{aligned} \quad (16)$$

For transition to the closed case one has only to replace  $H_0(t)$  by  $H(t, x(t))$  and add to the right side multiplier  $\exp \beta[F(x(0)) - F(x(t))]$ . It is easy to see that “quantum work FT” under this rule in fact coincides with (9)-(10).

In many applications of FDR one would like to connect the pair  $e^{-\beta H_0(t)} \dots e^{\beta H_0(0)}$ , - i.e. energy changes, - to some of variables  $A_k(t)$  under attention. In particular, when considering connections between fluctuations and non-linear responses at given ordering-symmetrization rule. Careful (though not complete yet) analysis of FDR (16) from such viewpoint was undertaken in [4].

9. In conclusion I should notice that the above considered relations can be extended to “thermic perturbations” [3] (i.e. non-equilibrium perturbations of initial state of the system, in addition to its Hamiltonian driving), thus expanding variety of FDR’s applications to non-equilibrium processes in open systems (see [2, 3] and references from [5]).

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- [1] G.N.Bochkov and Yu.E.Kuzovlev, “General theory of thermal fluctuations in nonlinear systems”, Sov.Phys.-JETP **45**, 125 (1977); [http://www.jetp.ac.ru/cgi-bin/dn/e\\_045\\_01\\_0125.pdf](http://www.jetp.ac.ru/cgi-bin/dn/e_045_01_0125.pdf)
- [2] G.N.Bochkov and Yu.E.Kuzovlev, “Fluctuation-dissipation relations for non-equilibrium processes in open systems”, Sov.Phys.-JETP **49**, 543 (1979); [http://www.jetp.ac.ru/cgi-bin/dn/e\\_049\\_03\\_0543.pdf](http://www.jetp.ac.ru/cgi-bin/dn/e_049_03_0543.pdf)
- [3] G.N.Bochkov and Yu.E.Kuzovlev, “Non-linear fluctuation-dissipation relations and stochastic models in non-equilibrium thermodynamics. I. Generalized fluctuation-dissipation theorem”, Physica **A 106**, 443 (1981).
- [4] Yu.E.Kuzovlev, “Fluctuation-dissipation relations for continuous quantum measurements”, arXiv: cond-mat/0501630.
- [5] Yu.E.Kuzovlev, “Short remarks on the so-called fluctuation theorems and related statements”, arXiv: 1106.0589.
- [6] M. Esposito, U. Harbola, and S. Mukamel, “Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems”, Rev. Mod. Phys. **81**, 1665 (2009).
- [7] D. Andrieux and P. Gaspard, Quantum work relations and response theory, Phys. Rev. Lett. **100**, 230404 (2008).
- [8] M. Campisi, P. Ha?nggi, and P. Talkner, “Colloquium: Quantum fluctuation relations: foundations and applications”, Rev. Mod. Phys. **83**, 771 (2011).
- [9] G.F.Efremov, “A fluctuation dissipation theorem for nonlinear media”, Sov. Phys. JETP **28**, 1232 (1969).
- [10] R.L.Stratonovich. Nonlinear nonequilibrium thermodynamics. Springer Series in Synergetics, Vol. 59. Springer-Verlag, Berlin.